CFD Analysis of Phase Holdup Behaviour in a Three Phase Fluidized Bed

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CERTIFICATE

This is to certify that the thesis entitled "**CFD analysis of Phase holdup behaviour in a Three Phase Fluidized Bed",** submitted by **Allada Chidambaram (107CH030)** to National Institute of Technology, Rourkela is a record of bonafide project work under my supervision and is worthy for the partial fulfillment of the degree of Bachelor of Technology (Chemical Engineering) of the Institute. The candidate has fulfilled all prescribed requirements and the thesis, which is based on candidate's own work, has not been submitted elsewhere.

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ABSTRACT

Fluidized beds are used extensively in various fields of engineering since they have the potential to promote high levels of contact between gases, liquids and solids. A characteristic set of basic properties of a fluidized bed can be practically used which is absolutely essential for the modern process and chemical engineering. Knowledge of the onset of fluidization is highly relevant and it serves as the key to three-phase fluidized-bed reactors design and safe operation. In a Three-phase fluidization the particulate solid is suspended in an upward co-current flow of gas and liquid. Three phase fluidized beds also commonly referred to as Gas-Liquid-Solid fluidized beds are used extensively in petrochemical, refining and food processing industries. The most important industrial application of the process is the heterogeneous catalytic hydrogenation of residual oils or coal slurry for the removal of sulfur and the production of hydrocarbon distillates by hydrocracking. Keeping in view the complexity of the hydrodynamic behavior of gas-liquid-solid fluidized, CFD analysis is used to predict the various characteristics.

In the present work FLUENT 6.3.26 has been used to study co-current gas-liquid-solid fluidization. CFD simulations have been done for a column of height 1.88 m and diameter 0.1 m containing glass beads as solid particles of size 2.18 mm. In the present work, involving three phase fluidized bed, CFD analysis of phase holdup behavior is studied. GAMBIT 2.3.16 has been used to generate a 2D coarse grid. Individual phase holdup have been determined in this present work. CFD results indicate that the gas as well as solid holdup increases with increasing gas velocity and decreasing liquid velocity. Liquid holdup increases with increasing liquid velocity and decreasing air velocity. The results have been compared with those calculated from the experimental work and have been found to agree well.

Keywords: Three phase fluidized bed, phase holdup, CFD

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NOMENCLATURE

g acceleration due to gravity, m sec^{-2}

k turbulent kinetic energy, J

t time

$M_{i,l}$ interphase force term for liquid phase

$M_{i,g}$ interphase force term for gas phase

$M_{i,s}$ interphase force term for solid

Greek Symbols

α_k volume fraction of phase k

v_m mass-averaged velocity

ρ_m mixture density, kg m^{-3}

ρ_k density of phase k = g (gas), l (liquid), kgm^{-3}

n number of phases

μ_{eff} effective viscosity

μ_m viscosity of the mixture, Pa s

μ_l liquid viscosity, Pa s

ε_k volume fraction of phase k = g (gas), l (liquid), s (solid)

ε rate of dissipation of turbulent kinetic energy, m^2s^{-3}

u_k velocity of phase k = g (gas), l (liquid), s (solid)

CHAPTER 1

INTRODUCTION

Fluidization is a process whereby a granular material is converted from a static solid-like state to a dynamic fluid-like state. This process occurs when a fluid (liquid or gas or both) is passed up through the granular material. If a fluid is passed through a bed of fine particles at a low flow rate, the fluid merely percolates through the void spaces between stationary particles. This condition is called the fixed bed. With an increase in flow rate, particles move apart and a few vibrate and move in restricted regions. This condition is called the expanded bed. At a still higher velocity, a point is reached where all the particles are just suspended by upward flowing fluid. At this point the frictional force between particle and fluid just counterbalances the weight of the particles, the vertical component of the compressive force between adjacent particles disappears, and the pressure drop through any section of the bed about equals the weight of fluid and particles in that section. The bed is considered to be just fluidized and is referred to as minimum fluidization. At this critical value, the bed is said to be fluidized and will exhibit fluidic behavior. When fluidized, a bed of solid particles will behave as a fluid, like a liquid or gas. (Levenspiel et al., 1991).

1.1 Gas-Liquid-Solid Fluidized Bed

In recent years gas-liquid-solid fluidizing beds have emerged as one of the most promising devices for three phase operations. They are considered immensely important in chemical and bio-chemical industries, treatment of waste water and other biochemical processes. Three phase fluidization mainly refers to the fluidization of solid particles by co-current upward flow of gas and liquid phase. It serves the purpose of bringing the three phases in contact in a single operation. In this type of reactor, gas and liquid are passed through a granular solid material at high enough velocities to suspend the solid in fluidized state. A porous plate called distributor supports the solid particles in the fluidized state at the static condition. It is through the distributor plate that the fluid is forced upwards through the solid material. Initially at lower fluid velocities the solid remains in place as the fluid passes through the voids in the material. Subsequently as the fluid velocity is increased, the bed reaches a stage where the force of the fluid on the solids is enough to balance the weight of the solid material. This stage is minimum fluidization and the corresponding fluid velocity is called minimum fluidization velocity. Once this minimum velocity is surpassed, the contents of the bed begin to expand and swirl around much like an agitated tank or boiling pot of water. The system can now be called a fluidized bed. (Howard., 1989).

The three phase reactors can be classified as slurry bubble column reactors and fluidized bed reactors depending upon the density and volume fraction of the particles. In a slurry bubble column the density of the particles is slightly higher than the liquid and size of particles range from 5-150 μm and volume fraction is below 0.15. The liquid phase along with the solid particles can be treated as the homogeneous liquid with mixture density. However in a fluidized bed reactors, the density of particles are much higher than the density of the fluid and particle size is normally large than 150 μm while the volume fraction of the solid particles varies from 0.6, in case of packed stage to 0.2 as in close transport stage (Paneerselvam et al., 2009)

1.2 Advantages of Gas-Liquid-Solid Fluidized Bed

The chief advantage of fluidization are that the solid particles are vigorously agitated by the fluid passing through the bed, and the mixing of the solid ensures that there are practically no temperature gradients in the bed even with quite exothermic or endothermic reactions. Some of the advantages are as follows (Heidari, 2007 and Kumar, 2009).

- The smooth, liquid-like flow of particles allows continuous automatically controlled operations with ease of handling.
- High rate of reaction per unit reactor volume can be obtained through these reactors.
- The rapid mixing of solids leads to nearly isothermal conditions throughout the reactor, hence the operation can be controlled simply and reliably.
- It is suited to large-scale operations.
- The circulation of solids between two fluidized beds makes it possible to transport the vast quantities of heat produced or needed in large reactors.
- Heat and mass transfer rates between gas and particles are high when compared with other modes of contacting.
- Benefits in economic, operational and environmental terms can be achieved with fluidized bed technology over traditional technologies.

1.3 Application of Gas-Liquid-Solid Fluidized Bed

In the last decade or so, application of fluidized bed has been important to various chemical industrial processes such as in pharmaceutical, metallurgical and mineral processing, in heat transfers, catalytic cracking, pyrolysis, combustion, etc. (Levenspiel et al., 1991). Fluidization has been used in many different processes, including the production of silicon for semiconductors and cultivation of micro-organisms in what has come to be called as "biofluidization" (Mahmood A., 2008). The gas-liquid-solid fluidized bed has emerged as one of the most promising devices for three phase operations Fluidized beds serve many purposes in industry, such as in the hydrogen –oil process for hydrogenation and hydrodesulphurization of residual oil, the H-coal process for coal liquefaction, and fischer-tropsch process (Jena et al., 2009).

Some of the commercial applications are as follows:

- Fluid catalytic cracking, reforming
- Fischer-Tropsch synthesis
- Catalyst regeneration
- Granulation (growing particles)
- Oxidation reactions involving solid catalyzed gas phase reactions
- Hydrotreating, hydroprocessing
- Biochemical processes
- Fluid coking
- Bio-oxidation process for waste water treatment
- Drying purposes (hot air drying of dolomite, coal grains)
- In transportation of solids like slurry pipeline for coal

1.4 Shortcomings of Three Phase Fluidized Bed

- It is difficult to describe flow of gas, with its large deviation from plug flow and bypassing of solids by bubbles results in an inefficient contacting system.
- The rapid mixing of solids in the bed leads to non-uniform residence time of solids in the reactor.
- For non-catalytic operations at high temperature the agglomeration and sintering of fine particles can necessitate a lowering in temperature of operation, resulting in the reduction of reaction rate (Lee ., 2002).
- Fluid like behavior of the fine solid particles within the bed results in abrasion leading to the erosion of pipes and vessels.

- Attrition of solids is one of the main disadvantages. Because of attrition, the size of the solid particles gets reduced and possibility for entrapment of solid particles with the fluid is more.

1.5 Modes of Operation of Gas-Liquid-Solid Fluidized Bed and Flow Regimes

Several types of operation for gas-liquid-solid fluidized bed are possible based on the differences in flow directions of gas and liquid and also based on the differences in the pattern of contact between the particles and the surrounding gas and liquid. The three phase fluidization can be classified into four modes of operation. These modes are as follows:

- Co-current three phase fluidization with liquid as the continuous phase.
- Co-current three phase fluidization with gas as the continuous phase.
- Inverse three phase fluidization.
- Fluidization by a turbulent contact absorber.

According to Epstein (1981), the liquid supported solid operation characterizes fluidization with the liquid velocity beyond the minimum fluidization velocity. The bubble supported solid operations characterizes fluidization with the velocity of liquid below the minimum fluidization velocity and hence it may be possible that the liquid is in stationary state.

Multiphase flow regimes can be grouped into four categories:

- Gas-liquid or liquid-liquid flows
- Gas-solid flows
- Liquid-solid flows
- Three phase flows

In this present work three phase flows is of prime importance which is actually the combination of the other flow regimes listed above it.

1.6 Variables Affecting the Quality of Fluidization

Variables which influence the quality of fluidization are as follows (Kumar, 2009):

- Fluid flow rate – Flow rate should be high enough to keep the solids in suspension but it should not be too much high that the fluid channeling occurs.
- Fluid inlet – Inlet must be designed in such a way that there is always well distribution of the fluid entering the bed.
- Particle size – Size of the particles greatly affect the quality of fluidization. Particles of different sizes are grouped into Geldart's classification of particles. Particles having a wide range are easier to fluidize than the particles of uniform size.
- Gas, liquid and solid densities – Closer is the relative density of the gas-liquid and the solid, easier is to maintain smooth fluidization.
- Bed height – With other variables remaining constant, it is more difficult to obtain good fluidization when the bed height is greater.

1.7 Need for CFD

Computational fluid dynamics is a whole new field which needs to be explored well. Over the recent years there have been various computational works but in comparison to the huge experimental data available, more works in the field of CFD is required. CFD predictions can be verified with the experimental data and results and can be checked if they hold good or not. With the experimental work being tedious, CFD helps in predicting the fluid flow, behavior of the fluidized bed and various hydrodynamic characteristics. CFD actually helps in modeling the prototype of a real world process and through CFD predictions one can apply those parameters to achieve the desired results. Thus the complex hydrodynamics of fluidization could be understood using CFD.

Objective of the work:

The aim of the present work could be summarized as follows:

- Study of complex hydrodynamics of gas-liquid-solid fluidized bed.
- Determining the individual phase holdup in a gas-liquid-solid fluidized bed.
- Analysis of the phase holdup behavior and various parameters that affect it.
- Examining the effect of superficial gas and liquid velocity on the individual phase holdup.

The present work is concentrated on understanding the phase holdup behavior in a three phase fluidized bed. Fluidized bed of height 1.88 m with diameter of 0.1 m has been simulated. Glass beads of diameter 2.18 mm are used as the solid phase. Co-current gas-liquid-solid fluidization has been done with the liquid (water) as the continuous phase. Liquid (water) and Gas (air) has been injected at the base with different superficial velocities. The static bed heights of the solid phase in the fluidized bed used for simulation are taken as 21.3 cm and 17.1 cm. In all the cases the initial holdup is taken to be 0.59 with the superficial velocity of gas varying from 0.0125-0.1 m/s and that of liquid ranging from 0.0-0.15 m/s. CFD simulations have been carried out using FLUENT 6.3, CFD Software. GAMBIT 2.3.16 has been used to design the Mesh.

1.8 Thesis Layout

The second chapter gives a comprehensive review of literature related to the hydrodynamic characteristics and phase holdup behavior. It includes the experimental as well as the computational aspect of gas-liquid-solid fluidization. The third chapter deals with the CFD methodologies for multiphase flows where the various basic approaches to the problem solution have been discussed. Computational flow model and the basic equations governing it have been discussed in chapter four. Chapter five deals with the result part obtained from simulations which have been discussed clearly. In chapter six (the last one) conclusions have been drawn on present work and scope of the future work has been presented.

CHAPTER 2

LITERATURE REVIEW

2.1 Scope

The fluidized bed is one of the best known contacting methods used in processing industry. There are many well established operations that utilize this technology. Three phase fluidized beds have been widely used in the polymer, chemical, petrochemical and biochemical industries.

The aim of this chapter is to give a comprehensive review of literature related to the hydrodynamic characteristics and phase hold up behavior in a gas-liquid-solid fluidized bed. An overview of the literature relevant to this study is presented next. The first section deals with the experimental works done and the succeeding section deals with the CFD predictions.

2.1.1 Experimental Review

A significant amount of experimental work has been done regarding the hydrodynamics and other characteristic behavior of fluidized bed. Various aspects have been considered ranging from the particle diameter to the fluid velocity. Earlier more emphasis was given on the hydrodynamics of a fluidized bed which dealt with the bed voidage, bed expansion, etc but recent studies have been done on the phase holdup, mass transfer in a fluidized bed, flow regime identification, etc. Various works on Gas-Liquid-Solid fluidization have been discussed below:

Soung Y. (1977) described three phase fluidization as a fluidization of solid particles by co-current upward flow of liquid and gas phase. Since it provides for contact between the phases in a multiphase flow systems, it has the advantage of superior heat transfer characteristics. He made an attempt to isolate the gas injection effect on the expansion of bed from the liquid viscosity. He even presented the correlations for the effect of gas velocity on bed expansion.

Kim et al. (1980) studied the phase holdup for beds of solids having binary size distributions, and correlated the phase holdup data empirically by the equations involving Reynolds and Froude numbers based on harmonic mean particle diameter. They examined that liquid phase holdups showed a decreasing trend with the subsequent increase in gas velocity and with decreasing liquid velocity. However, at higher gas velocities, liquid phase holdup is nearly independent of gas velocities, which may be due to the bubbly flow regimes progressed to intermediate or slug flow regimes with higher gas flow rates. Gas phase holdup increased with increasing gas velocity. Both the bed porosity and gas phase holdups increased with gas as well as liquid velocities.

For chemical processes where mass transfer is the rate limiting step, it is important to estimate the gas holdup, since this relates directly to the mass transfer, as concluded by Fan., (1989).

Lee and De Lasa (1987) investigated the bubble phase holdup and velocity in three phase fluidized beds. They used various operating conditions like elctroresistivity probe and optical fiber probe.

Muroyama and Fan, (1985) studied the behavior of a three phase fluidized bed and hence concluded that in a typical gas–liquid–solid three-phase fluidized bed, solid particles are fluidized primarily by upward concurrent flow of liquid and gas, with liquid as the continuous phase and gas as dispersed bubbles if the superficial gas velocity is low. Because of the good heat and mass transfer characteristics, three-phase fluidized beds or slurry bubble columns (u_t < 0.05 m/s) have gained considerable importance in their application in physical, chemical, petrochemical, electrochemical and biochemical processing.

Kim et al.,(1989) studied the phase holdup characteristics and bed porosity in three phase fluidized beds with a wide range of liquid properties and determined the effect of liquid and gas velocities, particle size, liquid properties such as viscosity and surface tension on the individual phase holdup and bed porosity in three phase fluidized beds. They concluded that liquid phase holdup increases with liquid velocity and viscosity, column diameter and liquid surface tension. It decreases with gas velocity, particle size and density difference between solid and liquid phases.

Krisnaiah et al. (1993) conducted experiments to study the hydrodynamics of three phase inverse fluidized beds using very light particles. Experimental data relating the minimum liquid velocity at the onset of fluidization was correlated in terms of particle characteristics, physical properties of fluids and system variables. He even proposed correlations for the friction factor.

Comte et al. (1997) studied the complex hydrodynamics of a three phase inverse turbulent bed and discussed about the critical gas velocity required to distribute the particles over the whole height of the reactor. They also discussed about the gas velocity required for uniform axial distribution of the solids.

After a thorough study on the hydrodynamics of gas-liquid-solid fluidized bed bio-reactor with a low density biomass support, Sokol and Halfani(1999) concluded that air holdup increases with increase in the inlet air velocity.

sivakumar et al. (2008) examined that the larger drag forces applied to the solid particles by an increase in liquid velocity cause an increase in liquid holdup. However for a constant liquid velocity, variation in liquid holdup with an increase of gas velocity was not significant. Liquid holdup decreases with an increase in particle diameter. Increase of particle sphericity reduces the surface area of particle per unit volume which leads more bubble breakage and hence liquid holdup decreases. At a constant fluid velocity, increase in liquid viscosity causes higher drag forces acting on the solid particles resulting in an increase in liquid holdup. Increasing liquid viscosity/fluid consistency index enhances the liquid interface and hence an increase in liquid holdup.

Schubert et al. (2009) worked on the phase holdups in three phase semi-fluidized bed and examined that the liquid saturation in the fixed bed increases with increasing superficial liquid velocity. For the same gas and superficial liquid velocities, the liquid saturation decreases with decrease in liquid kinematic viscosities. On the other hand opposite results were found for the gas saturation. The gas holdup in the fluidized bed is identified to be the most important and critical parameter.

2.1.2 Review of Computational Work

Computational Fluid Dynamics (CFD) that have been popular for quite a while in other fields of science (like space and mechanical engineering) and are becoming more and more interesting for chemical engineers. Experiments made way into computational analysis since experiments were tedious and time taking to perform. In computational fluid dynamics, advanced modeling approaches based on CFD techniques were applied for investigation of three phases in order to achieve accurate design and scale up. Some of the works are discussed below:

Bahary et al. (1994) used Eulerian multi-fluid approach for three-phase fluidized bed, where gas phase was treated as particulate phase having 4 mm diameter and a kinetic theory granular flow model was applied for the solid phase. They simulated both symmetric and axisymmetric model and verified the various flow conditions in the fluidized bed by comparing with the experimental data.

Schuteze et al. (1998) focused on CFD modeling of oxygen transfer in a stirred tank bioreactor and succeeded in even including the free surface into their mass transfer calculations.

CFD modeling results using CFX-4.2 for a randomly packed distillation column were presented by Yin et al. (2000). They compared their results to measurement data obtained at different

Operating conditions from a 1.22-m diameter, 3.66 m high packed bed that was equipped with several sizes of Pall rings. Good agreement with the predictions was achieved giving rise to the hope that CFD will become a useful tool for the scale-up of this class of apparatus as well. Similar computations have been carried out for semi-structured catalytic packed beds by Calis et al. (2001) using CFX-5.3. They found that pressure drop in such beds can be predicted with an error of less than 10 % compared to measurement results; still for such precision, very fine discretization grids (up to three million grid cells) and correspondingly high computational power is necessary.

Bauer and Eigenberger (2001) in their research paper called “Multiscale approach” described the fluid dynamics via CFD computation and included chemical reaction and mass transfer by means of a zone model.

Rusche (2002) investigated about the bubbles rising in a stagnant fluid and in a shear flow. A two-fluid (Euler-Euler) methodology was adapted to high phase fractions. Experimental data was used to verify the computational results. He concluded that computational results for air bubbles rising in quiescent water showed features like path instability and the shedding of wakes. Basically two types of trajectories were observed depending upon the bubble size. Bubbles with nominal diameter larger than 2mm prescribed a helical trajectory whereas smaller bubbles exhibit zigzag motion.

Joshi et al. (2002) determined the prediction of flow pattern near the wall and pressure drop in a bubble column reactor by using k-ε based model with low Reynolds number. Modeling of momentum transfer near the wall has been given special attention. The predicted and experimental hold-up and velocity profiles over wide range of column diameter, column height, bubble diameter and bubble rise show an excellent agreement.

Schallenberg et al. (2005) used 3-D, multi fluid Eulerian approach for three phase bubble column. Extended k-ε turbulence model were used to account for bubble induced turbulence and intherphase momentum between two dispersed phases were included. They validated the local gas and solid holdup as well as liquid velocities with the experimental data.

Paneerselvam et al. (2009) worked upon the CFD simulation of hydrodynamics of gas-liquid-solid fluidized bed reactor by developing a three dimensional transient model and compared the CFD simulation prediction with the experimental data of Kiared et al. (1999) which shows a good agreement. They also studied the influence of different interphase drag models for gas-liquid interaction on gas holdup.

Sivaguru et al. (2009) used CFD analysis to study the hydrodynamic characteristics of three phase fluidized bed. They developed a two dimensional simulation using porous zone and porous jump model. They found out that for uniform air-water flowrate, porous jump model is better than porous zone model. As the gas flowrate is increased with constant liquid flow rate, the pressure drop of the column decreases which is due to the reduced density in the bed since more gas holdup is there in the bed.

From the above literature review it is found that a lot of experimental work has been done in fluidization. Based upon the experimental results, many computational works have been verified. However many computational works are related in understanding the hydrodynamic behavior of a fluidized bed and very few are dedicated to the phase holdup analysis in three phase fluidized bed. From the previous studies it can be concluded that not much emphasis has been given on the phase holdup behavior. Hence an attempt is made in this present work to focus on the phase holdup behavior and to understand and completely analyze the phase holdup in a fluidized bed and also the various parameters upon which it depends.

CHAPTER 3

CFD METHODOLOGIES FOR MULTIPHASE FLOW

Multiphase flow is simultaneous flow of

- Materials with different states or phases (i.e. gas, liquid or solid).
- Materials with different chemical properties but in the same state or phase (i.e. liquid-liquid systems such as oil droplets in water).

Thus Multiphase flow refers to a situation where two or more fluids are present. Each fluid may have its own flow field, or all fluids may share a common flow field. One of the phases is continuous (primary) while the others (secondary) are dispersed within the continuous phase. A diameter has to be assigned for each secondary phase to calculate its interaction (drag) with the primary phase. A secondary phase with a particles size distribution is modeled by assigning a separate phase for each particle diameter. Each phase can be laminar or turbulent. Fluid flow (primary phase) may be turbulent with respect to the secondary phase but may be laminar with respect to the vessel (Bakker., 2002).

Multiphase flow is important in many industrial processes:

- Riser reactors
- Fluidized bed reactors
- Bubble column reactors
- Scrubbers, dryers, etc.

Typical objectives of a modeling analysis:

- Maximize the contact between the different phases, typically different chemical compounds.
- Flow dynamics.

This is where CFD (Computational Fluid Dynamics) comes into the picture in order to achieve the above said objectives of a multiphase flow.

3.1 CFD (Computational Fluid Dynamics)

CFD is a technology that enables us to study the dynamics of things that flow. Using CFD we can develop a computational model of the system or device that we want to study. Fluid flow physics is applied along with some chemistry and the software will output the fluid dynamics and the related physical phenomena. With the advent of CFD, one has the power to simulate the flow of gases and liquids, heat and mass transfer moving bodies, multiphase physics, chemical reaction, fluid structure interaction and acoustics through computer modeling. A virtual prototype of the system can be built using CFD (Fluent Inc, 2001). Thus CFD can applied for predicting the fluid flow associated with the complications of simultaneous flow of heat, mass transfer, phase change, chemical reaction, etc. using computers (Chaitanya .,2003). CFD has now become an integral part of the engineering design and analysis. Engineers can make optimal use of the CFD tools to simulate fluid flow and heat transfer phenomena in a system model and can even predict the system performance before actually manufacturing it (Ghoshdastidar., 1998).

3.2 Benefits of CFD

- Insight- if there is a device or system design which is difficult to analyze or test through experimentation, CFD analysis enables us to virtually sneak inside the design and see how it performs. CFD gives a deep perception into the designs. There are many occurrences that we can witness through CFD which wouldn’t be visible through any other means.

- Foresight- under a given set of circumstances, we can envisage through the CFD software what will happen. In a short time we can predict how the design will perform and test many variants until we arrive at an ideal result.
- Efficiency- the foresight we gain helps us to design better to achieve good results. CFD is a device for compressing the design and development cycle allowing for rapid prototyping.

Advantages of CFD can be summarized as (Ghoshdastidar ., 1998).

- The effect of various parameters and variables on the behavior of the system can be studied instantaneously since the speed of computing is very high. To study the same in an experimental setup is not only difficult and tedious but also sometimes may be impossible.
- In terms of cost factor, CFD analysis will be much cheaper than setting up experiments or building sample model of physical systems.
- Numerical modeling is flexible in nature. Problems with different level of complexity can be simulated.
- It allows models and physical understanding of the problem to be improved, very much similar to conducting experiments.
- In some cases it may be the only practicable ancillary for experiments.

3.3 CFD Process

The steps underlying the CFD process are as follows:

- Geometry of the problem is defined.
- Volume occupied by fluid is divided into discrete cells.
- Physical modeling is well-defined.

- Boundary conditions are defined which involves specifying the fluid behavior and properties at the boundaries.
- Equations are solved iteratively as steady state or transient state.
- Analysis and visualization of resulting solution is carried out.

3.4 Limitations of CFD

Even if there are many advantages of CFD, there are few shortcomings of it as follows (Bakker., 2002)

- CFD solutions rely upon physical models of real world processes.
- Solving equations on a computer invariably introduces numerical errors.
- Truncation errors due to approximation in the numerical models.
- Round-off errors due to finite word size available on the computer.
- The accuracy of the CFD solution depends heavily upon the initial or boundary conditions provided to numerical model.

3.5 Comparative Study of Experimental, Analytical and Numerical Methods

Experimental Method - experimental methods are used to obtain consistent information about physical processes which are not clearly understood. It is the most realistic approach for problem solving. It may involve full scale, small scale or blown up scale model. However disadvantages are high cost, measurement difficulties and probe errors.

Analytical Method - these methods are used to obtain solution of a mathematical model which consists of a set of differential equations that represent a physical process within the limit of conventions made. The systematic solution often contain infinite series, special functions etc. and hence their numerical evaluation becomes difficult to handle.

Numerical method – numerical prediction works on the results of the mathematical model. The solution is obtained for variables at distinct grid points within the computational field. It provides for greater handling of complex geometry and non-linearity in governing equations or boundary conditions. The kind of ease provided by numerical methods makes it the powerful and widely applicable. The above said discussion is represented in tabular form in table 3.1

Table 3.1. Comparison of Experimental, Analytical and Numerical Methods of Solution (Ghoshdastidar ., 1998)

Name of the Method	Advantages	Disadvantages
1. Experimental	Capable of being most realistic	• Equipment required • Scaling problem • Measurement difficulties • Probe errors • High operating costs
2. Analytical	Clean, general information which is usually in formula form	• Restricted to simple geometry and physics • Usually restricted to linear problems • Cumbersome results-difficult to compute
3. Numerical	No restriction to linearity. Ability to handle irregular geometry and complicate physics. Low cost and high speed of computation.	• Truncation and round-off errors • Boundary condition problems

An assessment of advantages and disadvantages of numerical methods vis-à-vis analytical and experimental method shows that even though the Numerical Method has few shortcomings but it has many advantages associated with it and is hence suited.

3.6 Approaches to Multiphase Modeling

The first step in solving any Multiphase problem is the selection of model. For a Multiphase flow there are two approaches for numerical calculations:

1. Euler-Lagrange approach
2. Euler-Euler approach

3.6.1 The Euler Lagrange Approach

This kind of approach is followed by the lagrangian discrete phase model. In this approach the fluid phase is treated as a continuous extent by solving the time averaged Navier-Stokes equations, while the dispersed phase is solved by computing a large number of particles, bubbles or droplets through the calculated flow-field. An altercation of momentum, mass and energy can take place between the dispersed phase and the fluid phase. Particle trajectories are computed individually at specified intervals during the fluid phase calculations and dispersed second phase occupies a low volume fraction which are the fundamental assumptions in this model. These assumptions make the model appropriate for spray dryers, coal and liquid fuel combustion and some particle laden flows but inappropriate for the modeling of liquid-liquid mixtures, fluidized beds or any application where volume fraction of second phase is negligible (Mohapatra and Rakh, 2007).

3.6.2 The Euler-Euler Approach

In this approach the concept of volume fraction is introduced based upon the fact that the volume of a phase cannot be carried or occupied by other phases. Here the different phases are treated mathematically as interpenetrating continua. The volume fractions are assumed to be continuous functions of space and time and their sum is equal to one. For each of the phase, conservation equations are derived to obtain a set of equations which have similar structure for all phases (Kumar, 2009).

The three different Euler-Euler Multiphase models available are

- The Volume of fluid (VOF) model
- The Mixture Model
- The Eulerian model

3.6.2.1 The VOF Model

The VOF model can model two or more immiscible fluids by solving a single set of momentum equations and tracking the volume fraction of each of the fluids throughout the domain. It is generally used to figure out a time dependent solution but for problems which are concerned with steady state solution, it is possible to perform a steady state calculation. A steady state VOF calculation is practical only when the solution is independent of the initial conditions and there are distinct inflow boundaries for the individual phases (Heidari, 2007)

3.6.2.2 The Mixture Model

The mixture model is designed for two or more phases (fluid or particulate). It is simplified multiphase model that can be used to model multiphase flows where the phases move at different velocities, but assume local equilibrium over short spatial length scales. It can also be used to model homogenous multiphase flows with very strong coupling and the phases moving at the same velocity. It is a good substitute for the full Eulerian multiphase model in several cases. It can model n phases by solving the momentum, continuity and energy equations for the mixture, the volume fraction equations for secondary phases and algebraic expression for the relative velocities (Heidari, 2007)

3.6.2.3 The Eulerian Model

The Eulerian model is the most complex among other multiphase models. It solves a set of n momentum and continuity equations for each phase coupling is achieved through the pressure and interphase exchange coefficients. The manner of handling of these couplings depends upon the type of phases involved. Granular (fluid-solid) flows are handled differently than non-granular (fluid-fluid) flows. For granular flows, the properties are obtained by applying kinetic theory (Kumar, 2009).

3.7 Choosing a General Multiphase Model

The first step in solving any problem is to determine which of the regimes provides some broad guidelines for determining the degree of interphase coupling for flows involving bubbles, droplets, or particles and the appropriate model for different amounts of coupling.

The appropriate model for flows involving bubbles particles or droplets are as follows (Heidari, 2007).

- For bubble, droplet and particle-laden flows in which dispersed-phase volume fractions are less than or equal to 10% the discrete phase model is to be used
- For bubble, droplet and particle-laden flows in which the phases mix and / or dispersed phase volume fractions exceed 10% the mixture model is used.
- For slug flow, the VOF model is used.
- For stratified / free-surface flows, VOF model is used.
- For fluidized bed, Eulerian Model for granular flow is used.
- For slurry flows and hydro transport, Eulerian or Mixture model is used.

CHAPTER 4

CFD SIMULATION OF GAS-LIQUID-SOLID FLUIDIZED BED

4.1 Computational Flow Model

Eulerian multi-fluid model is adopted in the present work where gas and liquid phases are all treated as continuous, inter-penetrating and interacting everywhere within the computational domain. The pressure filed is assumed to be shared by all the three phases proportional to their volume fraction. The motion of each phase is governed by the respective mass and momentum equations. Heidari (2007) discussed that Eulerian multiphase model in FLUENT allows for the modeling of multiple distinct yet interacting phases. With the Eulerian multiphase model, the number of secondary phases is limited only by memory requirements and convergence behavior. Any number of secondary phases can be modeled, if sufficient memory is available.

4.1.1 Equations

Continuity Equation:

$$\frac{\partial}{\partial t}(\rho_m) + \nabla.(\rho_m\, v_m) = 0$$

Where v_m is the mass-averaged velocity

$$v_m = \left(\sum_{k=1}^{n} \alpha_k\, \rho_k\, v_k \right) / \rho_m$$

ρ_m is the mixture density:

$$\rho_m = \sum_{k=1}^{n} \alpha_k\, \rho_k$$

α_k is the volume fraction of phase k

Momentum Equation:

For liquid phase:

$$\frac{\partial}{\partial t}(\rho_l \varepsilon_l u_l) + \nabla.(\rho_l\, \varepsilon_l\, u_l\, u_l) = -\varepsilon_l \nabla p + \nabla.(\varepsilon_l\, \mu_{eff,l}(\nabla u_l + \nabla u_l^{T})] + \rho_l\, \varepsilon_l\, g + M_{i.l}$$

For gas phase:

$$\frac{\partial}{\partial t}(\rho_g \varepsilon_g u_g) + \nabla.(\rho_g\, \varepsilon_g\, u_g\, u_g) = -\varepsilon_g \nabla p + \nabla.(\varepsilon_g\, \mu_{eff,g}(\nabla u_g + \nabla u_g^{T})] + \rho_g\, \varepsilon_g\, g + M_{i,g}$$

For solid phase:

$$\frac{\partial}{\partial t}(\rho_s \varepsilon_s u_s) + \nabla.(\rho_s\, \varepsilon_s\, u_s\, u_s) = -\varepsilon_s \nabla p + \nabla.(\varepsilon_s\, \mu_{eff,s}(\nabla u_s + \nabla u_s^{T})] + \rho_s\, \varepsilon_s\, g + M_{i,s}$$

Where μ_{eff} is the number of phases, $M_{i.l}$, $M_{i,g}$, $M_{i,s}$ represent the interphase force term for liquid, gas and solid phase respectively.

4.1.2 Turbulence Modeling

The choice of turbulence model will depend upon (Heidari, 2007):

- Physics encompassed in the flow
- The established practice for a specific class of problem
- The level of accuracy required
- The available computational resources
- Amount of time available for simulation

To make the most appropriate choice of model one must understand the capabilities and limitations of the various options. In the present work standard k-ε model is chosen for modeling the turbulence. k-ε is a turbulence model on the basis of RANS (Reynolds-Average Navier-Stokes) approach and has been developed by Launder and Spalding in 1972. The turbulence model is a set of equations which expresses relations between unknown terms appearing in the Reynolds-averaged governing quantities. The k-ε model focuses on the mechanisms that affect the turbulent kinetic energy and is nearly homogeneous. In the derivation of k-ε model, the assumption is that the flow is fully turbulent and the effects of molecular viscosity are negligible

(Spalding et al., 1972). Analytical expressions are used to bridge the wall boundary and the fully turbulent fluid since the choice of the k- ε standard wall function determines that the viscosity affecting the near wall region is not resolved. The expression implemented in FLUENT is the logarithmic law of the wall for velocity. Wall functions avoid the turbulence model adaptation to the presence of the wall, saving computational resources. (Kumar, 2009).

4.1.3 Phase Holdup

The phase holdup is the fraction of individual phase occupied in three phase contacting and is one of the most important parameter to determine the hydrodynamic properties of gas-liquid-solid fluidized beds (Mahmood, 2008).

Since the sum total of the entire individual phase holdup is equal to one, it can be stated as:

$\varepsilon_l + \varepsilon_s + \varepsilon_g = 1$, where

ε_l is the holdup of continuous (water)

ε_s is the holdup of solid (particles)

ε_g is the holdup of dispersed (air)

4.2 Problem Description

The problem comprises a three phase fluidized bed in which air and water enters at the bottom of the column. The bed consists of solid material (glass beads) of uniform diameter which is filled in the column up to a preferred height. The following table 4.1 shows the properties of air, water and glass beads used.

Table 4.1 Properties of air, water and glass beads used in the experiment

Phases	Density	Viscosity
Air	1.225 kg/m^3	1.789*10^{-05} kg/m-s
Water	998.2 kg/m^3	0.001003 kg/m-s
Glass beads	2470 kg/m^3	0.001003 kg/m-s

4.3 Simulation

4.3.1 Geometry and Mesh

Gambit 2.3.16 was used for making 2D rectangular geometry with width of 0.1 m and height 1.88 m. Coarse mesh size of 0.01 m was taken in order to have 1880 cells (3958 faces) for the whole geometry. Smooth mesh can be created taking mesh size of 0.005 m. But in case of smooth mesh the iterations per time step increases, hence a coarse grid mesh is preferred.

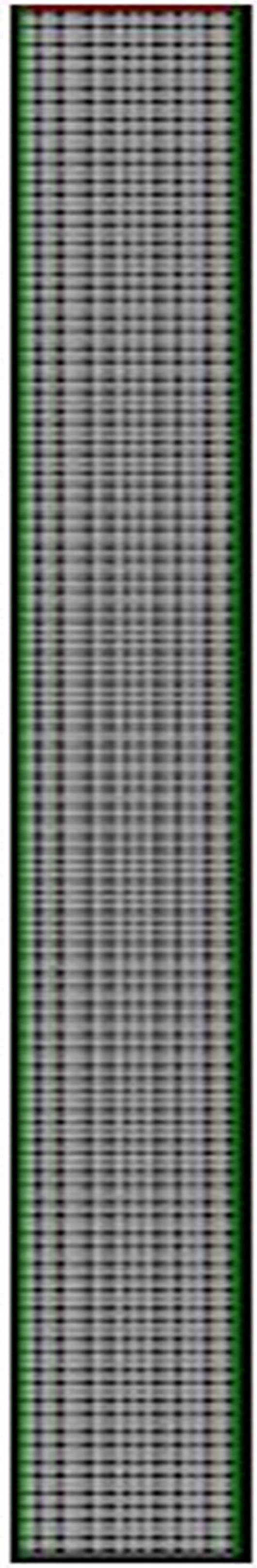


Fig.1. Mesh Created in Gambit

4.3.2 Selection of Models for Simulation

FLUENT 6.3.26 was used for simulation. 2D segregated 1st order implicit unsteady solver is used. Standard k-ε dispersed Eulerian multiphase model with standard wall functions were used for modeling turbulence. The value of various model constants is tabulated as:

Table 4.2 Model constants used for simulation

Model Constants	Value
Cmu	0.09
C1-Epsilon	1.44
C2-Epsilon	1.92
C3-Epsilon	1.3
TKE Prandtl Nummber	1
TDR Prandtl number	1.3
Dispersion Prandtl Number	0.75

Water is taken as the primary phase which is the continuous phase while glass beads and air as dispersed phase. Inter-phase interactions formulations used for Drag Coefficient were

- Air-Water: Schiller-Naumann
- Glass beads-Water: Gidaspow
- Glass beads- Air: Gidaspow

Air velocities ranging from 0.0125 m/s to 0.1 m/s with increment of 0.0125 and water velocities from 0 to 0.15 m/s with increment of 0.03 were used respectively. The inlet air volume fraction was obtained as the fraction of air entering in the mixture of gas and liquid.

Pressure outlet boundary conditions:

Mixture Gauge Pressure- 0 Pascal

Solid and Liquid Boundary Conditions:

Backflow granular temperature- 0.0001 m^2/s^2

Backflow Volume Fraction- 0

Specified Shear Stress was set as X=0 and Y=0 for gas and solid whereas for water no slip condition was used.

4.3.3 Solution

The under relaxation factor for solution control in different flow quantities were taken as pressure = 0.3, Density = 1, Body Forces = 1, Momentum = 0.3, Volume Fraction = 0.5, Granular Temperature = 0.2, turbulent Kinetic Energy = 0.8, Turbulent Dissipation Rate = 0.8, Turbulent Viscosity = 1. Pressure- Velocity Coupling was chosen as Phase Coupled SIMPLE. First Order Upwind was chosen for Discretization. The solution has been initialized from all zones. For patching a solid volume fraction, volume fraction of the solid in the part of the column up to which the glass beads were fed, was used. Iterations were carried out for time step size of 0.01-0.001 liable on the ease of convergence and the time required to achieve the fluidization results. The following figure shows the residual plot for k-ε solver method as the iteration proceeds.

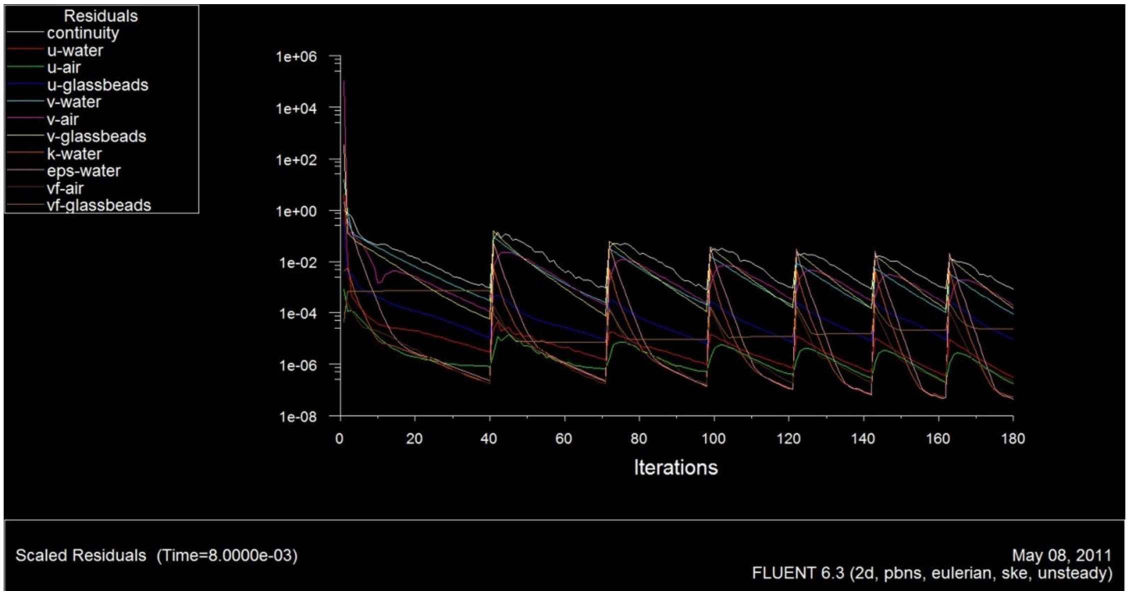


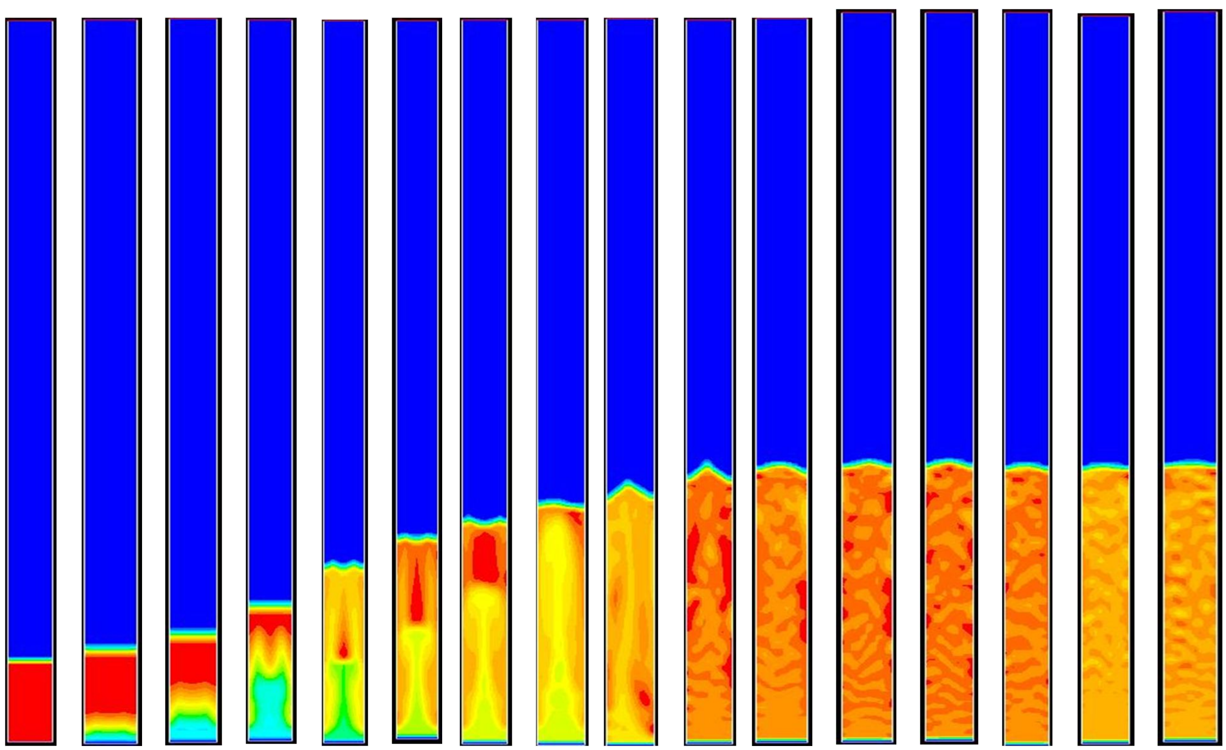
Fig.2 Plot of Residuals for k-ε solver method as the iteration proceeds

A convergence criterion of 0.001 has been used in the simulation. While simulating, the profile of the bed changes. For a longer physical flow time, the simulations are carried out till the solution reaches a Quasi-steady state.

CHAPTER 5

RESULT AND DISCUSSION

A gas-liquid-solid fluidized bed of diameter 0.1m and height 1.88 m has been simulated using commercial CFD software package FLUENT 6.3.26. Static bed of heights 17.1 cm and 21.3 cm has been used for simulation. Diameter of the glass beads (solid phase) were taken to be 2.18 mm. Inlet superficial velocity of gas were taken in a range of 0.0125m/s to 0.1m/s while that of water were taken in the range of 0 to 0.15 m/s. The simulation results obtained have been shown graphically in the following figure 3.

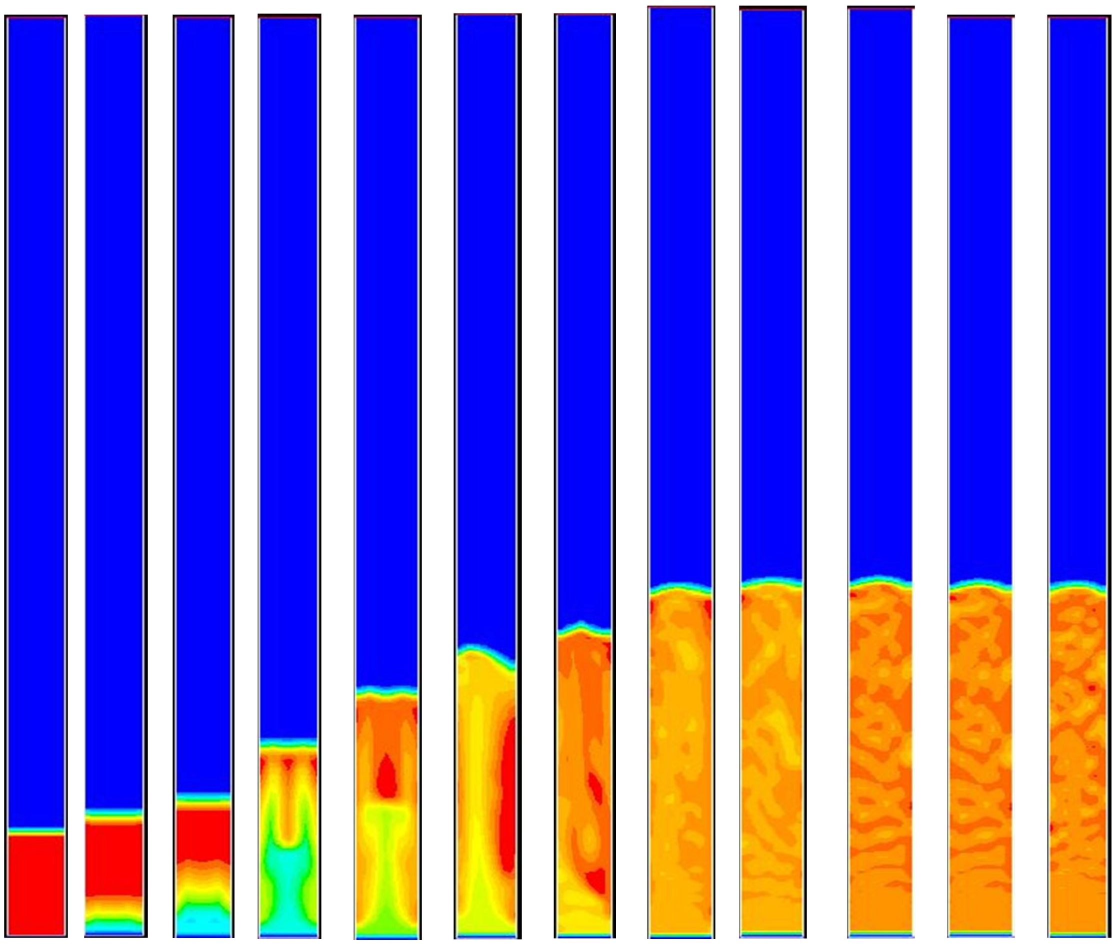


0 0.5 1 2 4 6 8 10 12 15 18 21 25 30 35 40

sec sec sec sec sec sec sec sec sec sec sec sec sec sec sec sec

Fig.3. Contours of volume fraction of glassbeads at water velocty of 0.12m/s and air velocity of 0.025m/s for initial bed height of 21.3 cm.

While simulation takes place, a change in profile is seen in the column, but after some time no significant change is observed which indicates that the quasi steady state has been reached. Simulations were carried out till there was no change in the bed profile. From the figure it is very much clear that the bed profile changes for the first 25 sec, after which there is no subsequent change in the bed profile even though the simulation goes on, like that between 25 to 40 seconds.



0 sec	0.5 sec	1 sec	2.5 sec	5 sec	7.5 sec	10 sec	15 sec	18 sec	21 sec	23 sec	25 sec

Fig.4. Contours of volume fraction of glass beads at water velocity 0.12 m/s and air velocity 0.025 m/s for initial bed height of 17.1 cm.

Here the quasi steady state is reached in the first 25 seconds.

5.1 Phase Dynamics

Solid, liquid and gas phase dynamics have been represented in the form of contours, vectors and XY Plot. Figure 4 shows the contours of volume fraction of solid, liquid and gas in the column obtained at water velocity of 0.12m/s and air velocity of 0.025m/s for static bed height of 21.3 cm after the quasi steady state is achieved. The colour scale given to the left of each contour indicates the value of volume fraction corresponding to the colour.

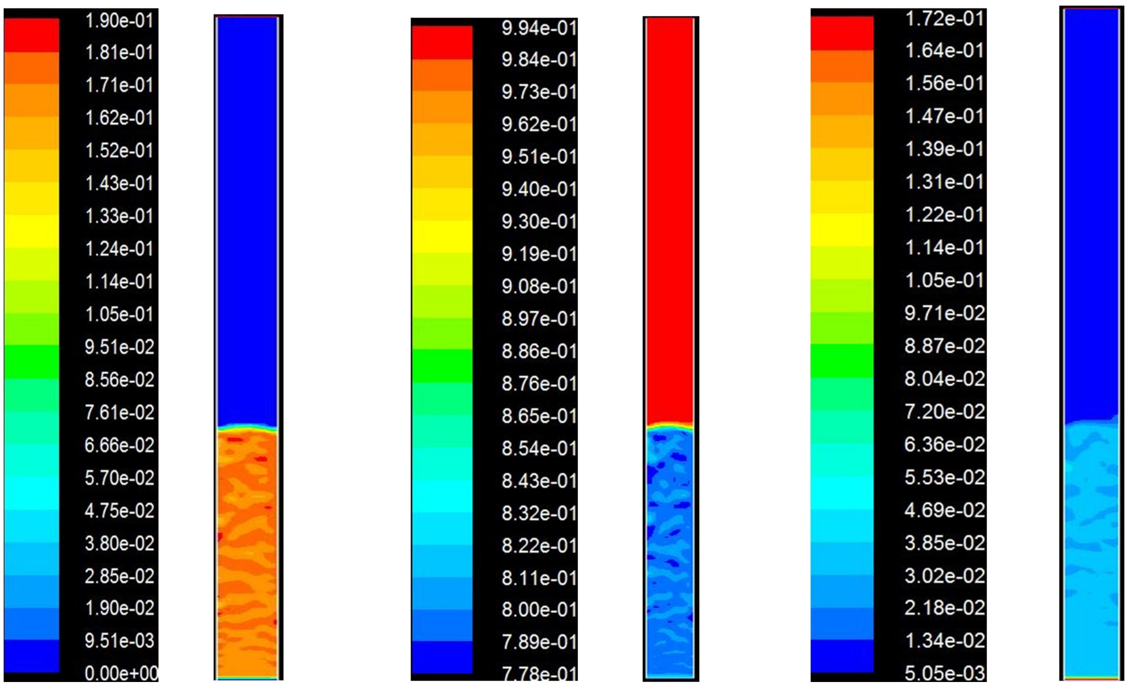


Fig.5. Contours of volume fractions of solid, liquid and gas at a water velocity of 0.12 m/s and air velocity of 0.025 m/s for initial bed height of 21.3 cm.

The contour for glassbeads shows that the bed is in fluidised condition. Contour for water shows that volume fraction of water is less in fluidized part of the column in comparion to the rest part of the column. The gas holdup is more in fluidzed part of the bed as illustrated by the contours for air.

Vectors of velocity magnitude of glass beads, water and air in the column obtained at inlet water velocity of 0.12m/s and inlet air velocity of 0.0125m/s for static bed height 21.3 cm are show in the following figures.

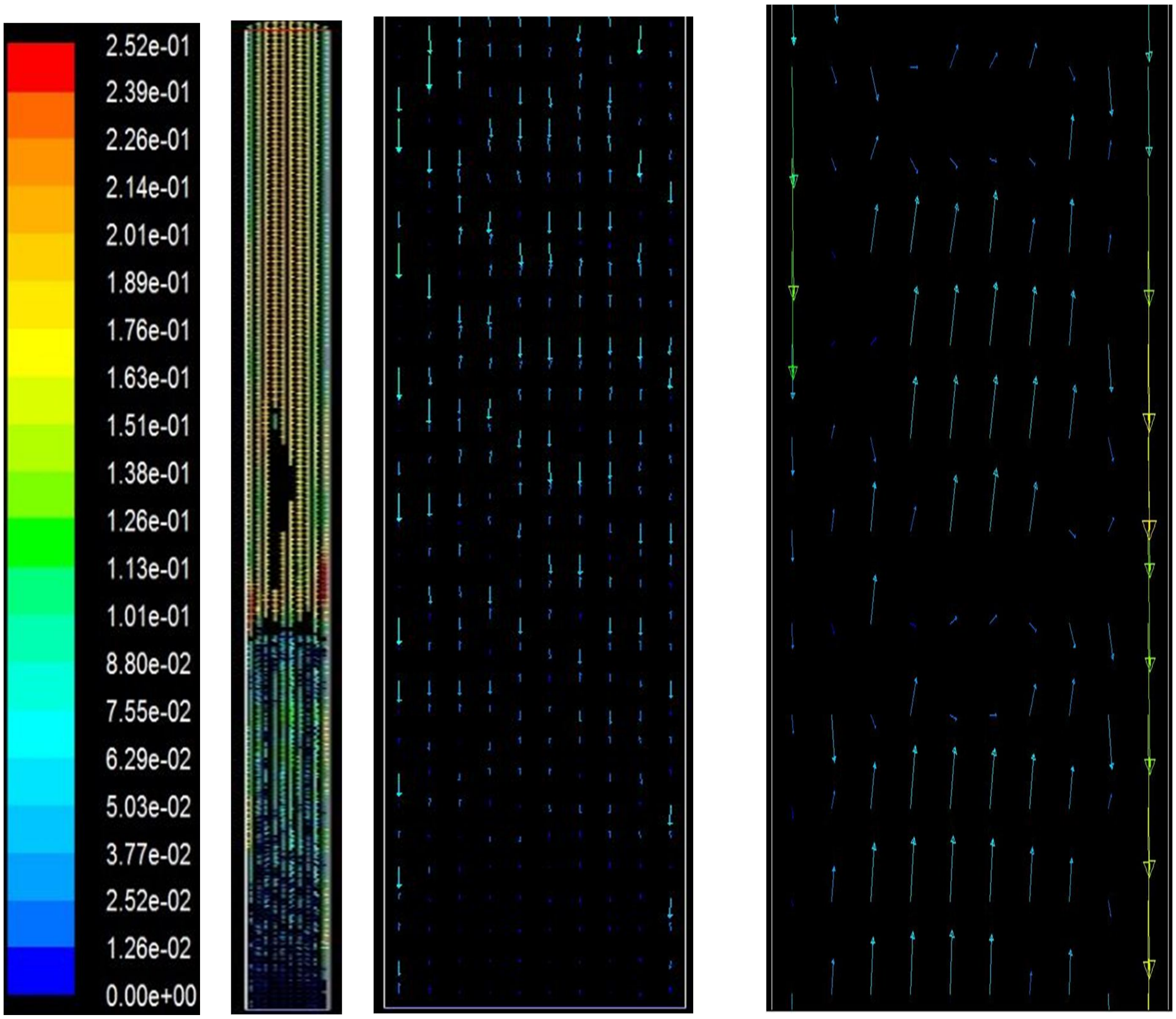


Fig.6. Velocity vectors of glass beads in the column, (actual view and magnified view)

It is very much evident from the picture that the velocity at the bottom is small. At the top expanded part of the bed the velocity vectors show a downward trend and since no glassbeads are present at the top, no velocity vectors are seen. At the middle portion the direction of velocity of the particles show downward trend but that of the particles away from the wall is vertically upwards.

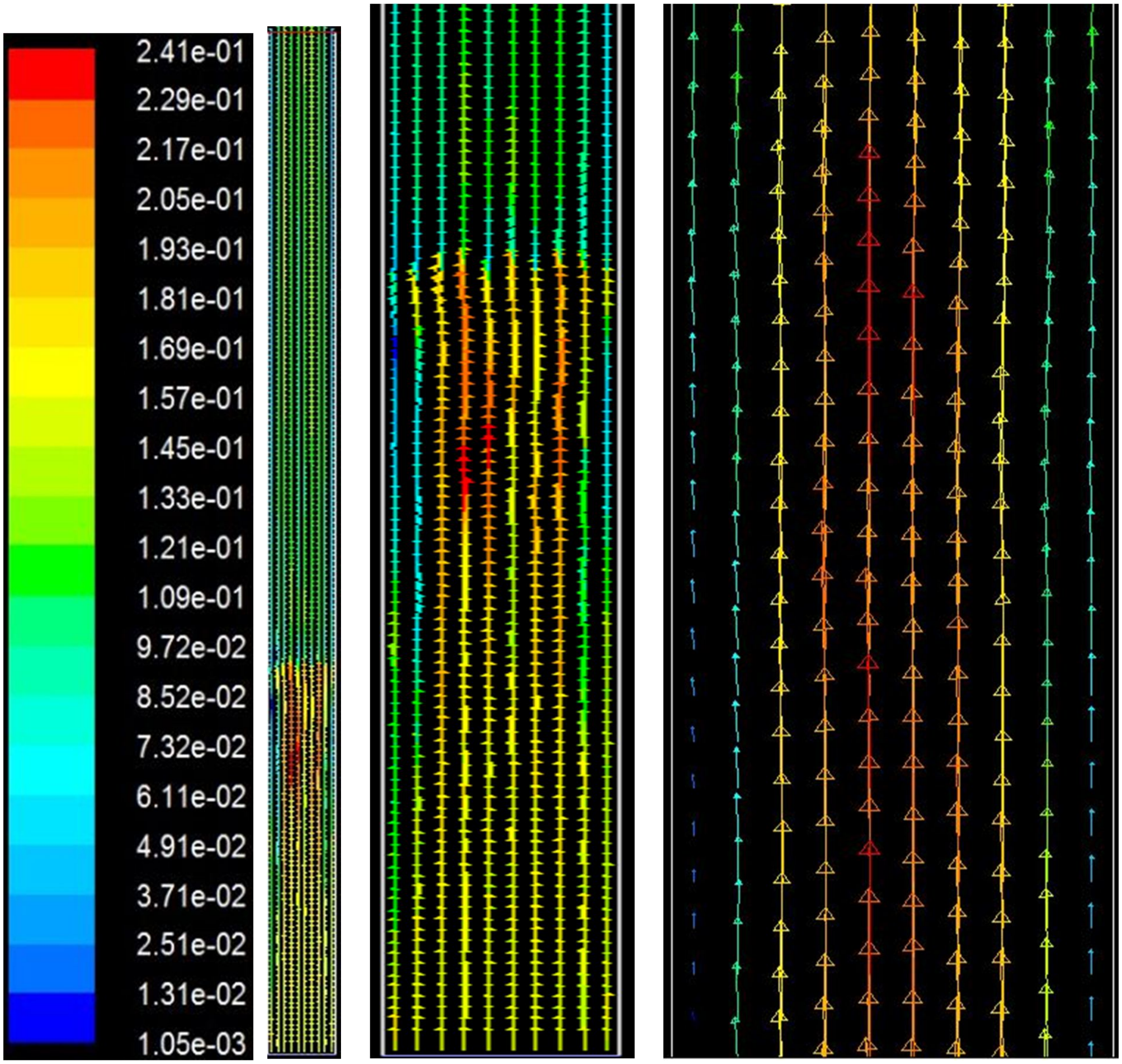


Fig.7. Velocity vector of water in the column (actual view and magnified view)

Velocity vector of water shown an upward trend throughout. However velocity is more in the fluidized part of the column compared to the part where there is no glass beads. The reason is that the flow of liquid faces an obstruction in the fluidized section of the bed where glassbeads are present.

The following figure 8 shows the velocity vector of air. It is evident from the figure that the velocity of air is very small in the fluidized part of the column.

The reason is that volume fraction of air is very less compared to that of glass beads and water in the fluidized part of the column. Moreover the flow of air bubbles is restricted by the glass beads present in the bed.

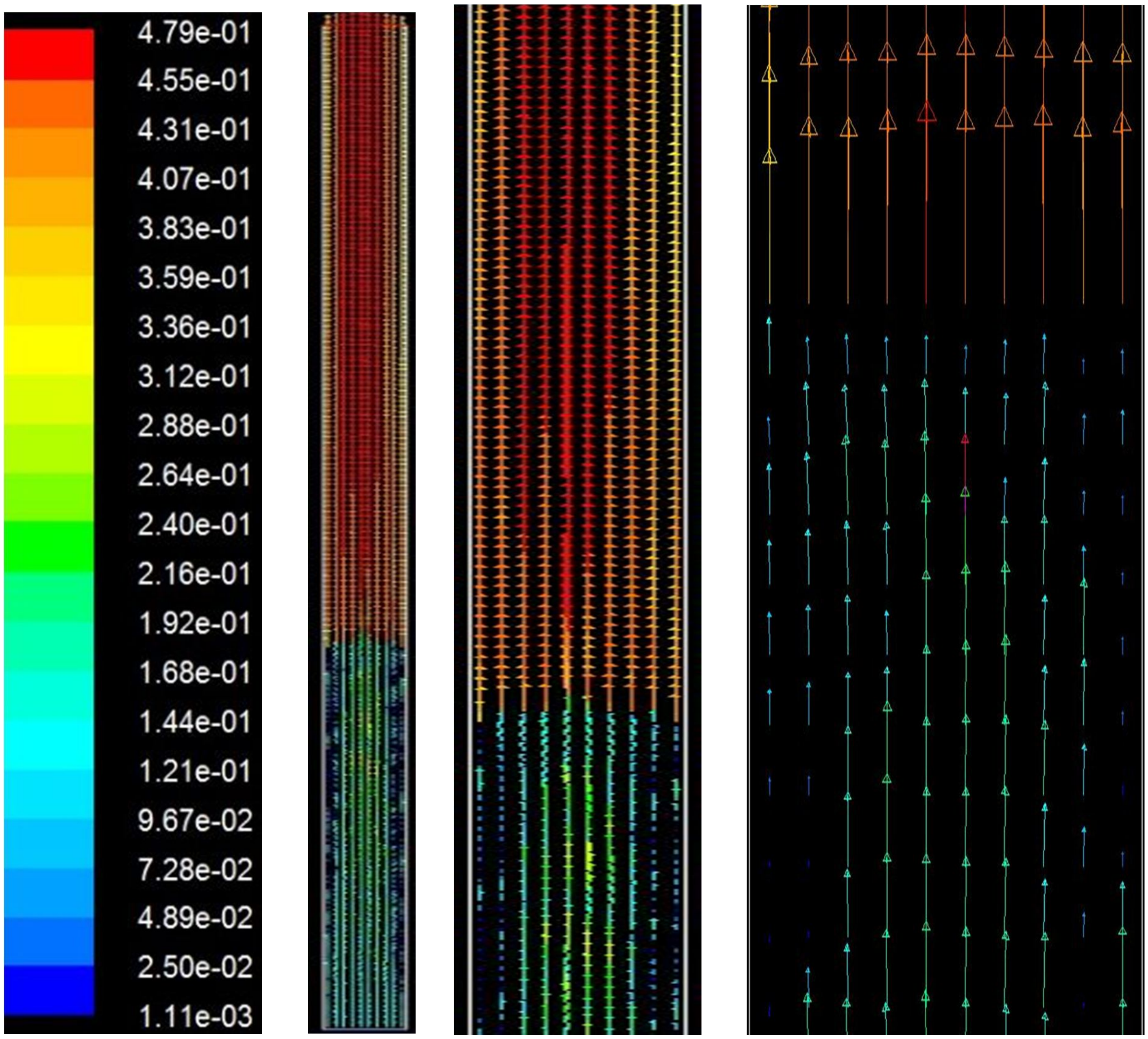


Fig.8. Velocity vector of air in the column (actual view and magnified view)

In the upward section of the column, it may also be possible that the high water velocity carries the air bubble along with them, so their velocity decreases.

Following figure 9 and figure 10 show the XY Plot of velocity magnitudes of air and water obtained at an inlet air velocity of 0.025m/s and water velocity 0.12m/s. A parabolic curve is obtained in the plot which a necessary pattern for a fully developed flow.

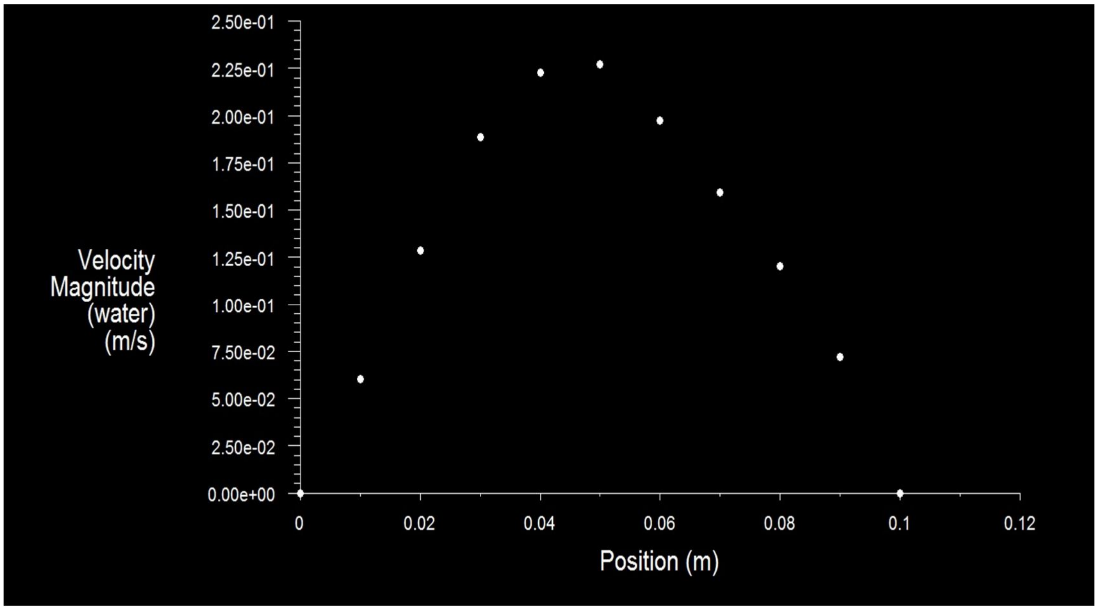


Fig.9. XY plot of velocity magnitude of water

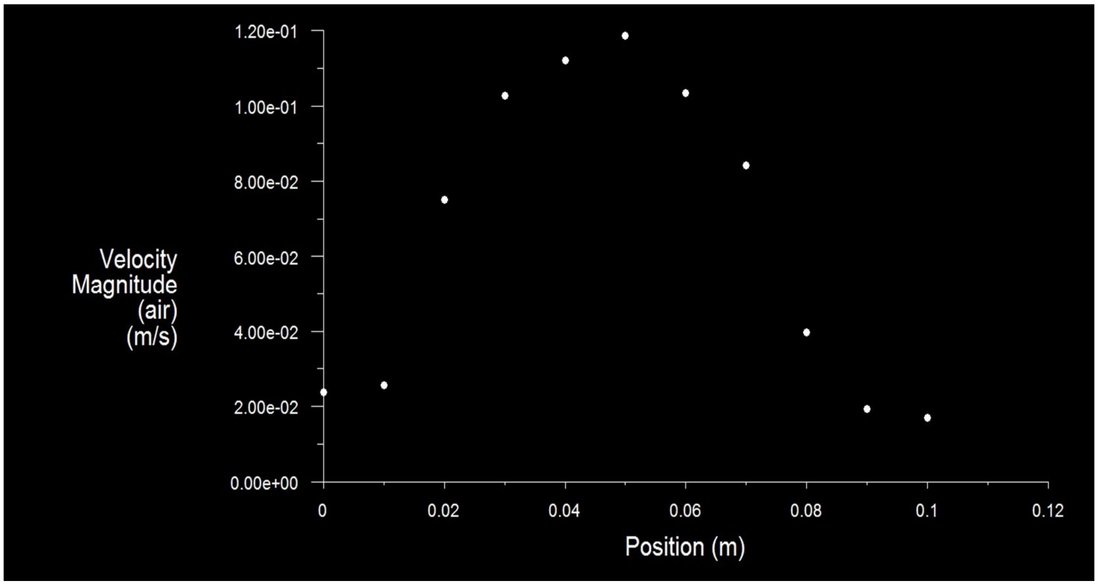
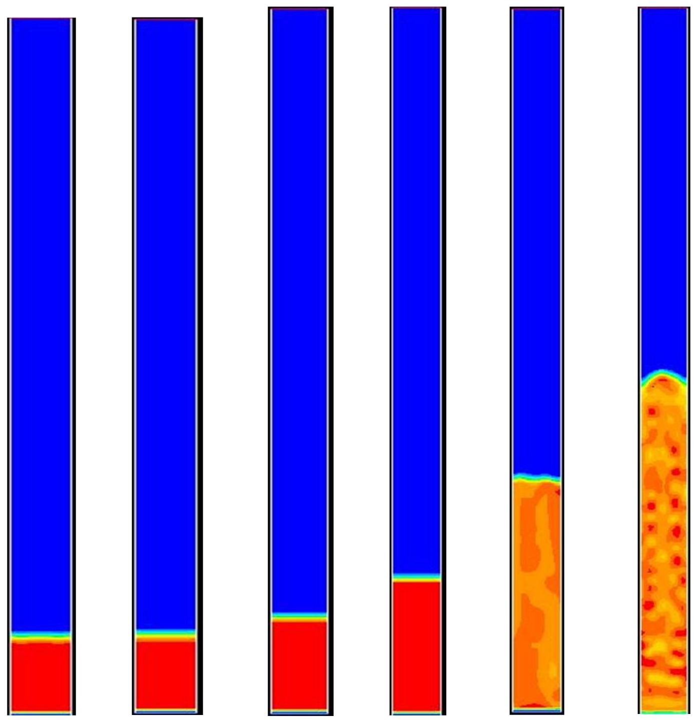


Fig.10. XY plot of velcoity magnitude of air.

5.2 Bed Expansion

The following figure shows the contours of the volume fraction of glassbeads at an inlet air velocity of 0.075 m/s and different water velocities for static bed height of 21.3 cm and glass beads of size 2.18 mm. The figure clearly shows that the bed epands as liquid velocity is increased at constant gas velocity.



Water velocity (m/s) 0.0 0.03 0.06 0.09 0.12 0.15

Fig.11. Contours of the volume fraction of glass beads with increasing water velocity at inlet air velocity of 0.075 m/s for initial bed height of 21.3 cm.

Thus the figure shows that bed expands when liquid velocity is increased at constant air velocity. At higher velocity of water the bed expansion is vigorous as illustrated by the above figure.

5.2.1 Bed Height

Bed height is determined from the X-Y plot of volume fraction of glass beads on Y-axis and height of the column on X-axis.

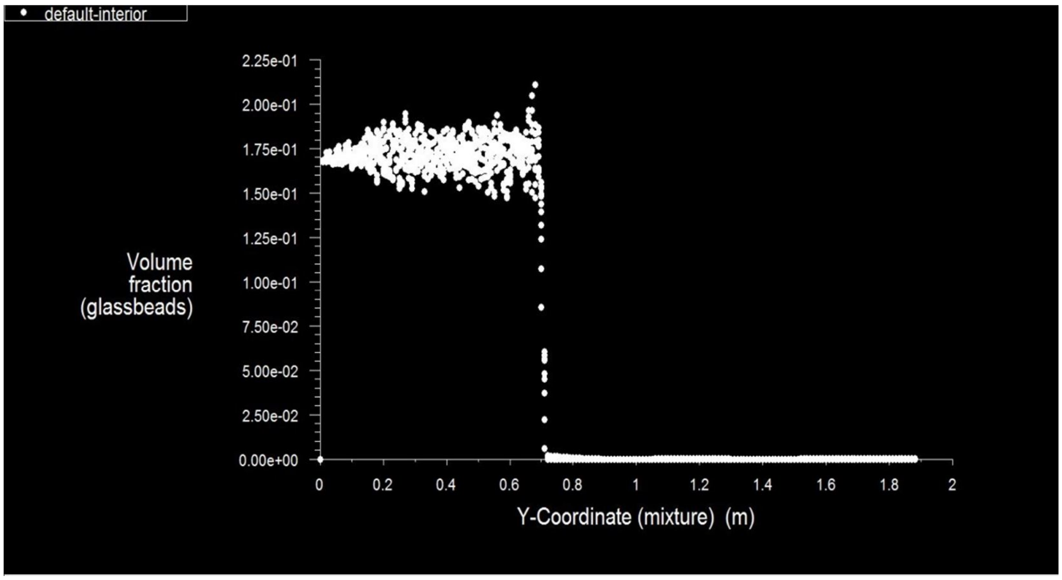


Fig.12. XY plot of glass beads at an air velocity of 0.025m/s and water velocity of 0.12m/s

Even from the XY plot, one can predict the bed height observing at the Xaxis (Y-coordinate mixture) and also the volume fraction of the glassbeads corresponding to the height shown in Y-axis.

The variation in the nature of bed height at varying water and air velocity have been shown in the following figures.

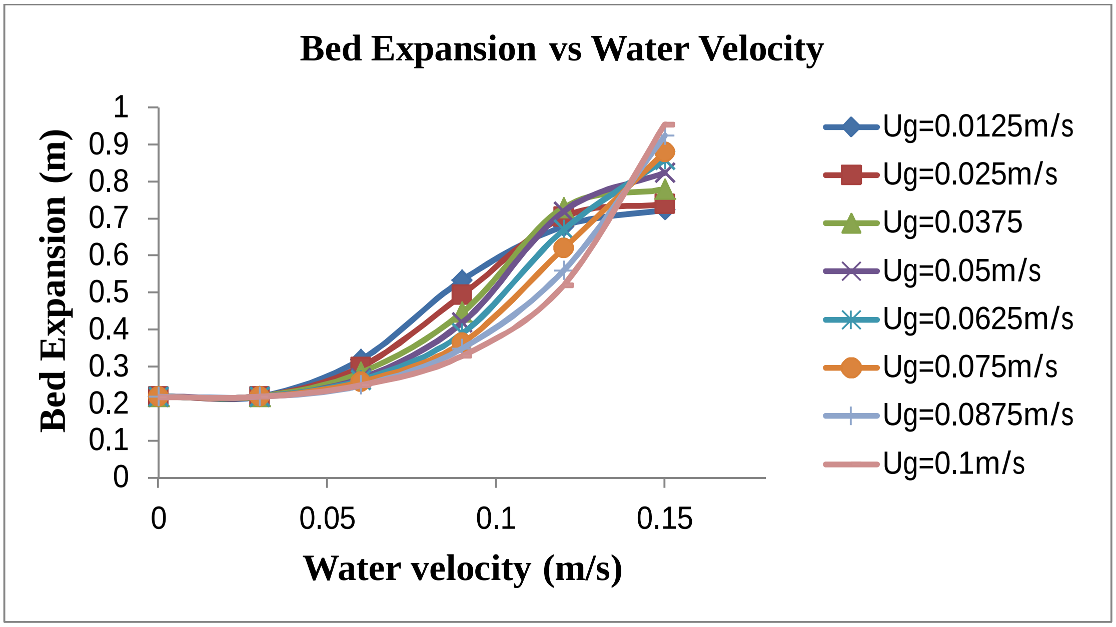


Fig.13. Bed Expansion vs Water velocity for initial bed height of 21.3 cm

The above figure illustrates that bed height shows an increasing trend as the water velocity is increased for a particular air velocity.

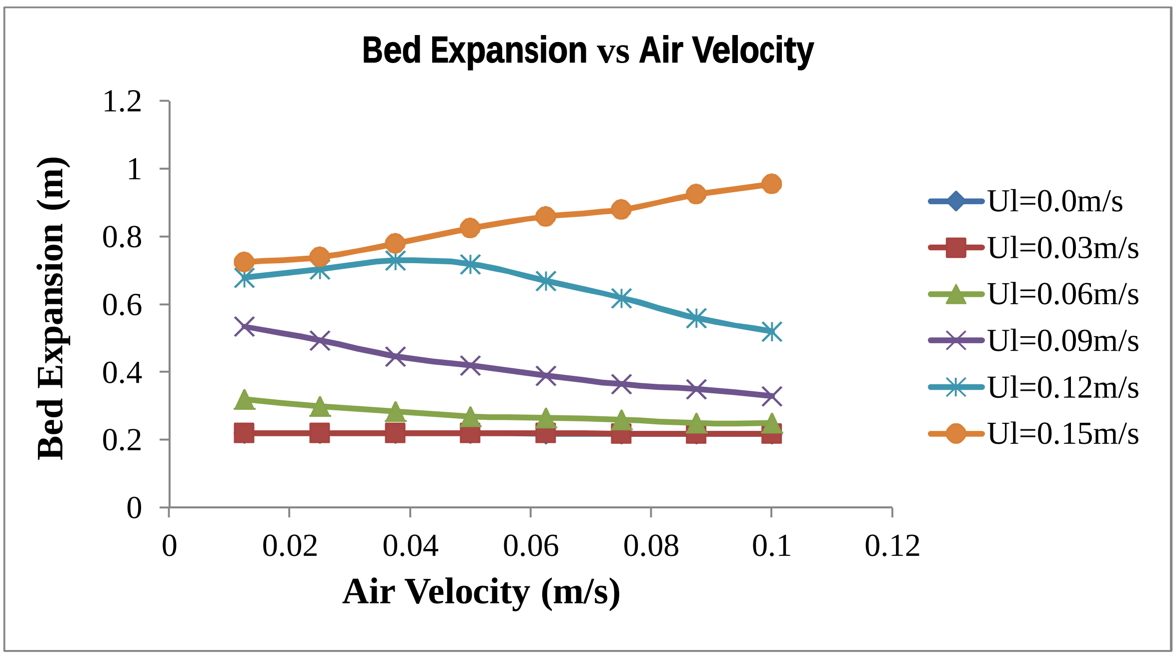


Fig.14. Bed Expansion vs Air Velocity for bed height of 21.3 cm

It is observed from the above figure that for a particular velocity of water, when the air velocity is subsequently increased there is a decrease in the bed height. This trend is more significantly observed at lower velocities of water. Particles of dia. less than 2.58 mm show an increasing bed expansion at higher liquid velocities. The same behavior can be observed here as the bed height increases for water velocity 0.15m/s. The bed height also increases at liquid velocity 0.12 m/s but only for air velocity 0.0125 m/s and 0.025 m/s and then it shows a decreasing trend as observed in other lower cases of liquid velocity.

5.3 Phase Holdup

Individual phase holdup and their behavior with varying water and air velocity have been discussed in this section and illustrated nicely through figures.

5.3.1 Gas Holdup

Gas hodup is obtained as mean-area weighted average of volume fraction of air at sufficient number of points in the fluiidzed part of the bed. Since the volume fraction of air phase is not the same at all points in the fluiidzed part of the column, hence an area weighted average of volume fraction of air determined at regular height till the fluidized part is over. When these values are averaged it gives the required gas holdup. Here an area weighted average of volume fraction of air is determined at heights 10 cm, 20 cm, 30 cm etc. The following figure 15 shows the plot of gas holdup varying with subsequent change in water velocity.

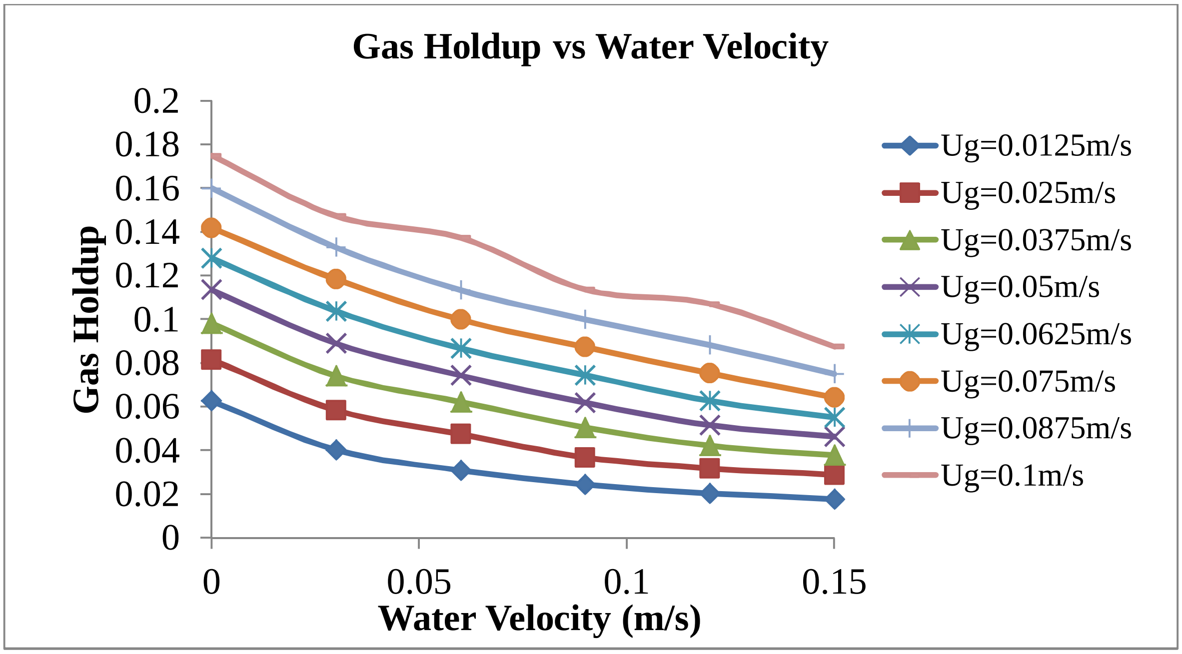


Fig.15. Gas holdup vs Water Velocity for initial bed height of 21.3 cm

It is observed from the plot that for a particular air velocity, the gas holdup decreases with the increase in water velocity.

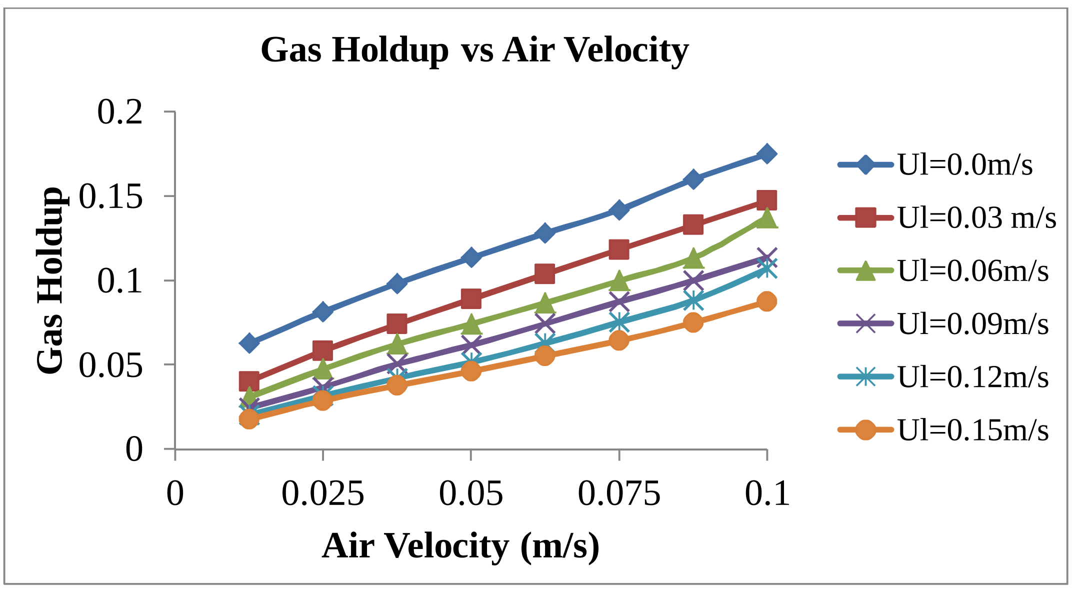


Fig.16. Gas holdup vs Air Velocity for initial bed height of 21.3 cm

Keeping the water velocity constant, it is observed that the gas holdup increases monotonically with the increase in air velocity.

5.3.2 Liquid Holdup

Following are the plots showing liquid holdup.

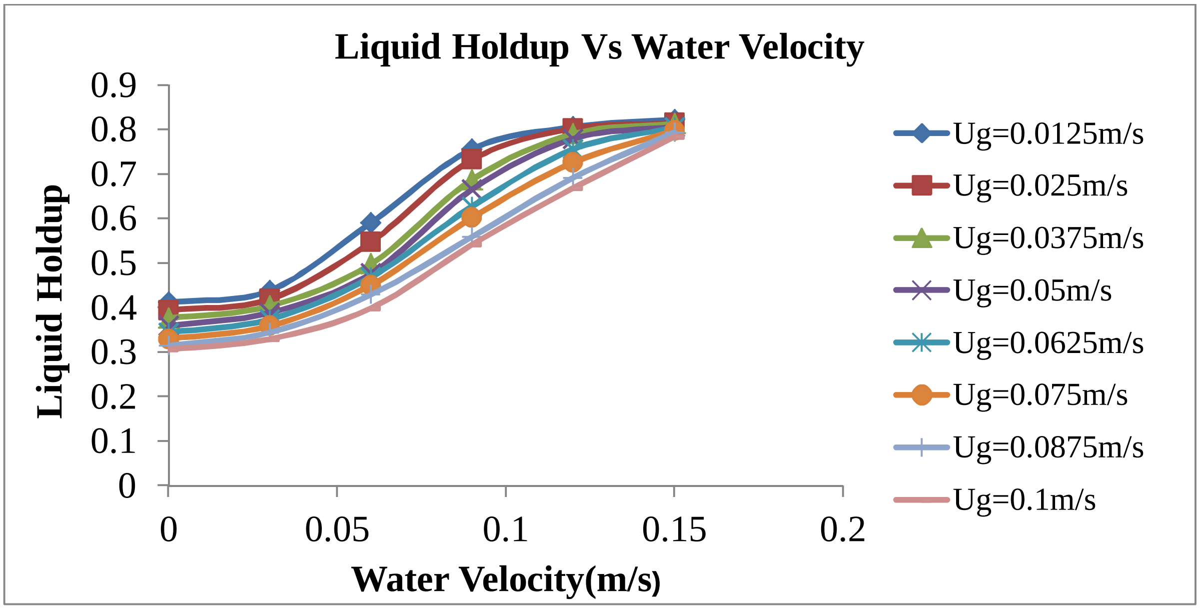


Fig.17. Liquid holdup vs Water Velocity for initial bed height of 21.3 cm

It is observed from the previous plot that liquid holdup increases with the increase in water velocity at a given velocity of air.

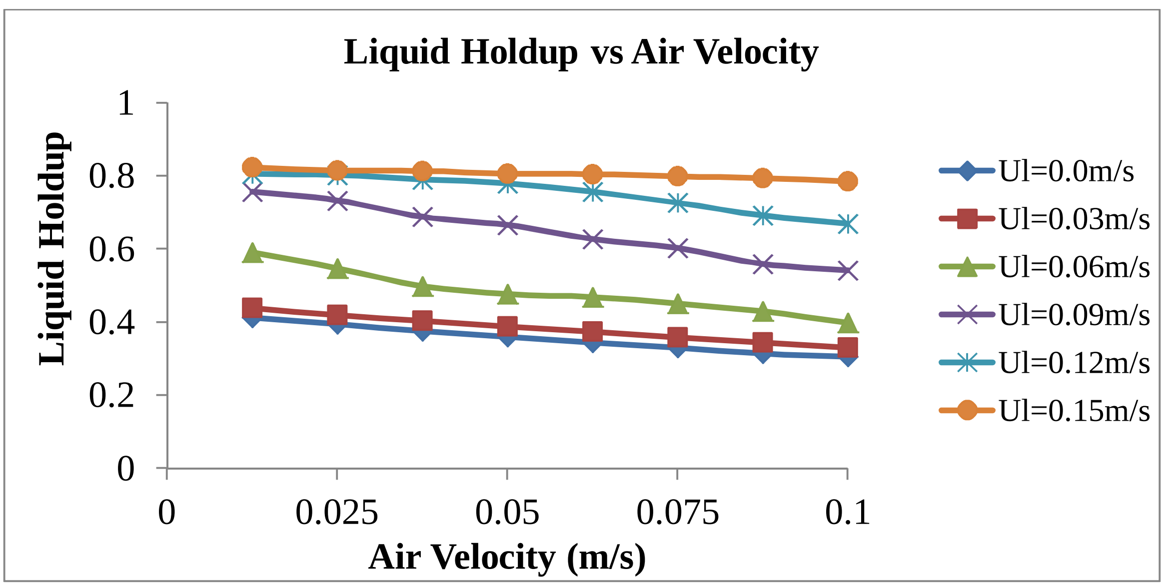


Fig.18. Liquid Holdup vs Air Velocity for initial bed height of 21.3 cm

From the plot in figure 19, it is observed that for a given water velocity, the liquid holdup decreases as the inlet air velocity is increased. For water velocity lying in the range of 0.06m/s to 0.12 m/s, the decreasing trend is more in comparison to the much lower velocities.

5.3.3 Solid Holdup

It shows a trend opposite to the bed expansion. Following figures show the variation in solid holdup with varying inlet water velocity and air velocity.

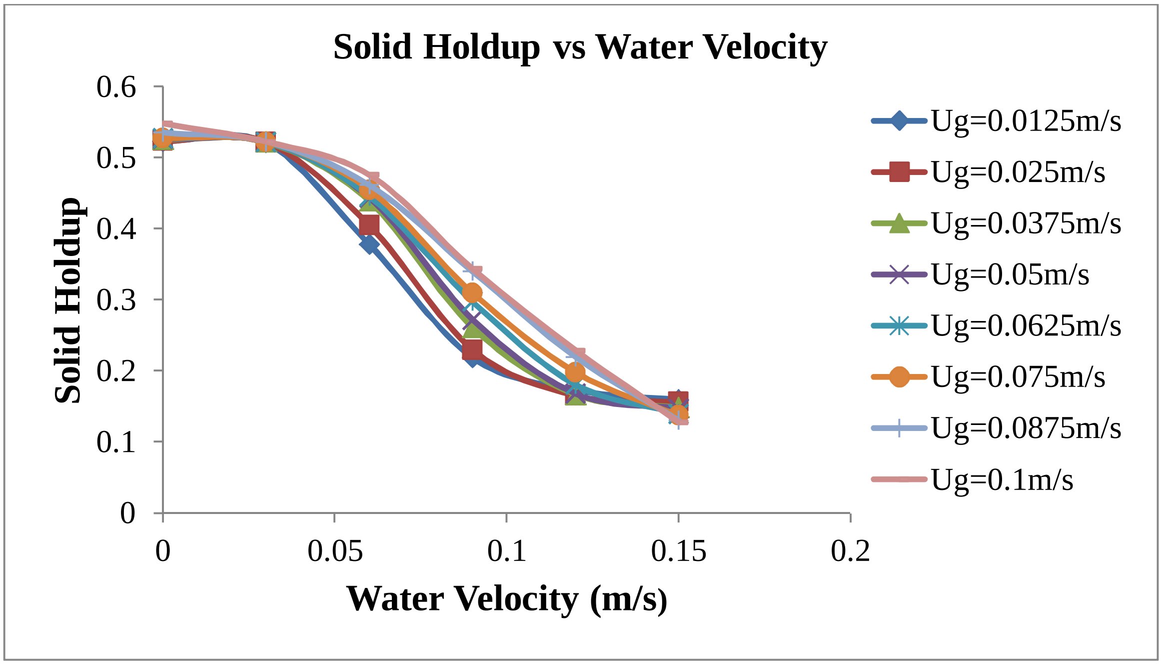


Fig.19. Solid Holdup vs Water Velocity for initial bed height of 21.3 cm

From figure 19 it is clear that the solid holdup decreases with increase in inlet water velocity. This corresponds to the same trend in which the expanded bed height decreases with the increase in water velocity as discussed earlier.

Next is shown the variation of solid holdup with the air velocity.

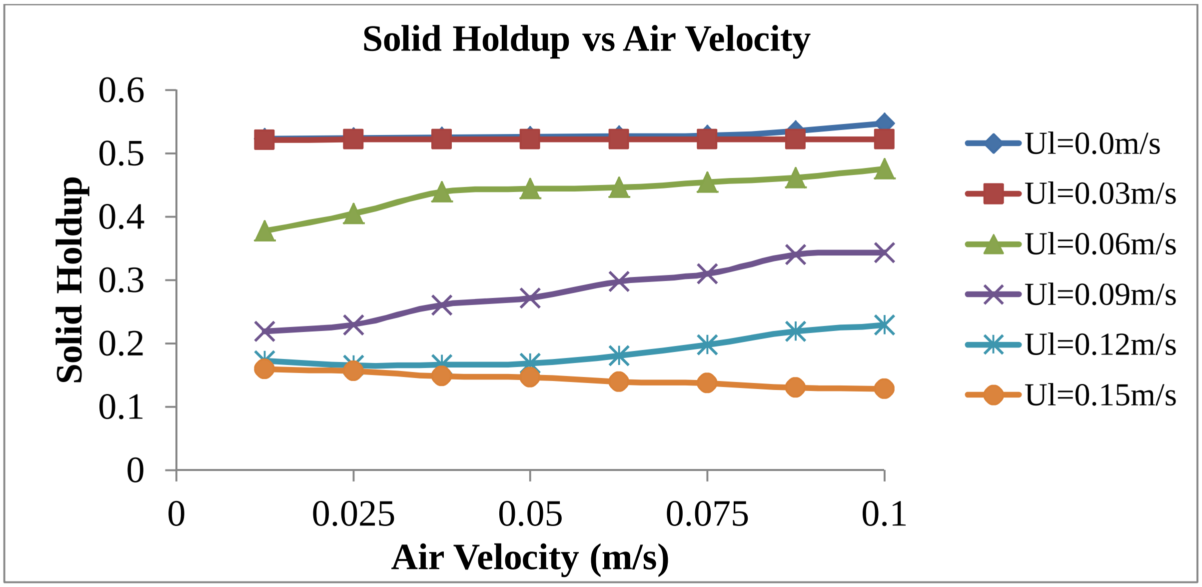


Fig.20. Solid Holdup vs Air Velocity for initial bed height of 21.3 cm

It is seen that solid holdup increases with increase in air velocity corresponding to water velocity ranging from 0.0 m/s to 0.12 m/s. At higher water velocity of 0.15 m/s, solid holdup decreases as air velocity is increased since the bed expansion takes place and hence the volume fraction of the glass beads (solid phase) decreases.

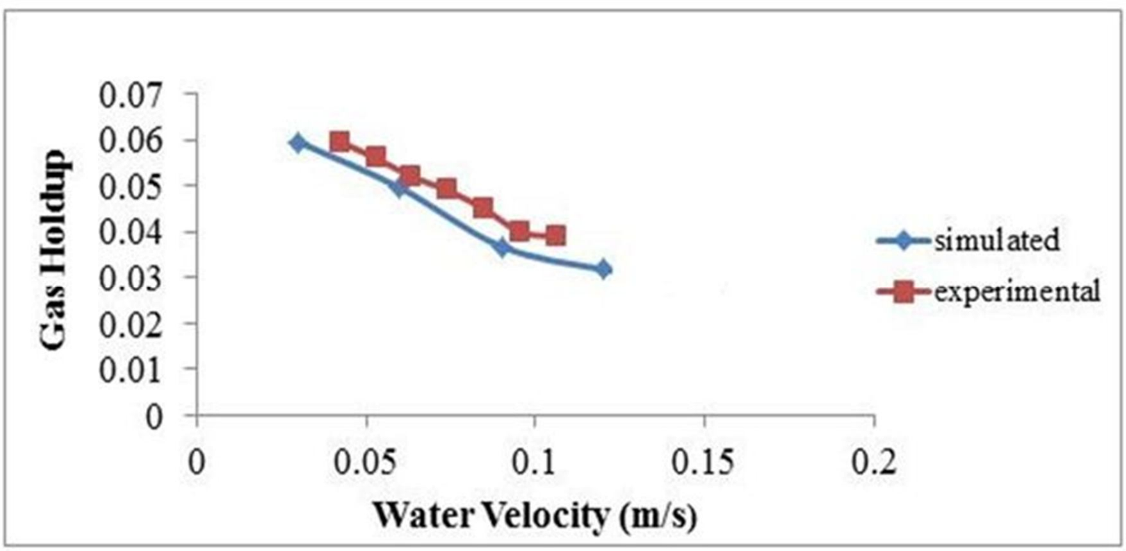


Fig.21.Comparision of experimental result of gas holdup with that of the simulated result obtained at inlet air velocities of 0.0625m/s for initial bed height of 21.3 cm.

The above plot shows comparison of experimental result of gas holdup with that of simulated result obtained at air inlet velocities 0.0625 m/s for initial bed height 21.3 cm. The simulated results have been compared with the experimental results of Jena et al (2009).It shows that simulated results are in excellent agreement with experimental results with deviation of less than 9%. The reason for deviation may be that the glass beads used in experiment have a range of diameters while in the simulation all glass beads are taken to be of the same diameter.

CHAPTER 6

CONCLUSION

6.1 Conclusion

CFD simulations of gas-liquid-solid fluidized bed were carried by employing Eulerian -Eulerian approach for different operating conditions. In three phase fluidization the hydrodynamic variables studied were gas, liquid and solid holdup, bed expansion, XY plots and velocity vectors. The three phase interactions which are very complex and time consuming in experiments have been studied in this present work. The main aim was to analyze the individual phase holdup behavior in a three phase fluidized bed.

Main conclusions that can be drawn are:

- Contour of volume fraction of water shows that the volume fraction of water is less in fluidized part of the column in comparison to the rest part.
- Gas holdup is more in fluidized part of the bed as illustrated by the contours for air.
- Bed expands when liquid velocity is increased at constant air velocity as illustrated from the plot of bed expansion vs liquid velocity. For low inlet velocity of water, the bed height decreases with the subsequent increase in air velocity.
- Trends of Gas Holdup vs inlet Air velocity shows that gas holdup increases with increase in air velocity obtained at different inlet water velocities.
- Trends of liquid holdup vs inlet Water Velocity show that liquid holdup increase with the increase in inlet water velocity at different inlet velocities of air.
- Solid holdup obtained decreases with the increase in inlet water velocity at different inlet velocity of air.

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